

**(19)F spin-lattice relaxation of perfluoropolyethers: Dependence on temperature and magnetic field strength (7.0-14.1T).**

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**Public Summary:**

Fluorine ((19)F) MRI of perfluorocarbon-labeled cells has become a powerful technique to track the migration and accumulation of cells in living organisms. It is common to label cells for (19)F MRI with nanoemulsions of perfluoropolyethers that contain a large number of chemically equivalent fluorine atoms. Understanding the mechanisms of (19)F nuclear relaxation, and in particular the spin-lattice relaxation of these molecules, is critical to improving experimental sensitivity. To date, the temperature and magnetic field strength dependence of spin-lattice relaxation rate constant ( $R_1$ ) for perfluoropolyethers has not been described in detail. In this study, we evaluated the  $R_1$  of linear perfluoropolyether (PFPE) and cyclic perfluoro-15-crown-5 ether (PCE) at three magnetic field strengths (7.0, 9.4, and 14.1T) and at temperatures ranging from 256-323K. Our results show that  $R_1$  of perfluoropolyethers is dominated by dipole-dipole interactions and chemical shift anisotropy.  $R_1$  increased with magnetic field strength for both PCE and PFPE. In the temperature range studied, PCE was in the fast motion regime ( $\omega\tau_c \ll 1$ ) at all field strengths, but for PFPE,  $R_1$  passed through a maximum, from which the rotational correlation time was estimated. The importance of these measurements for the rational design of new (19)F MRI agents and methods is discussed.

**Scientific Abstract:**

Fluorine ((19)F) MRI of perfluorocarbon-labeled cells has become a powerful technique to track the migration and accumulation of cells in living organisms. It is common to label cells for (19)F MRI with nanoemulsions of perfluoropolyethers that contain a large number of chemically equivalent fluorine atoms. Understanding the mechanisms of (19)F nuclear relaxation, and in particular the spin-lattice relaxation of these molecules, is critical to improving experimental sensitivity. To date, the temperature and magnetic field strength dependence of spin-lattice relaxation rate constant ( $R_1$ ) for perfluoropolyethers has not been described in detail. In this study, we evaluated the  $R_1$  of linear perfluoropolyether (PFPE) and cyclic perfluoro-15-crown-5 ether (PCE) at three magnetic field strengths (7.0, 9.4, and 14.1T) and at temperatures ranging from 256-323K. Our results show that  $R_1$  of perfluoropolyethers is dominated by dipole-dipole interactions and chemical shift anisotropy.  $R_1$  increased with magnetic field strength for both PCE and PFPE. In the temperature range studied, PCE was in the fast motion regime ( $\omega\tau_c \ll 1$ ) at all field strengths, but for PFPE,  $R_1$  passed through a maximum, from which the rotational correlation time was estimated. The importance of these measurements for the rational design of new (19)F MRI agents and methods is discussed.

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